LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061016\
Data File : BG022289.D
Acq On : 10 Jun 2016 15:43
Operator : UM/SJ
Sample : H3438-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.973 | 17 | 23 | 42 | rVB | 425491 | 786455 | 61.44% | 8.739% |
| 2 | 5.176 | 392 | 398 | 408 | rBV2 | 17071 | 32615 | 2.55% | 0.362% |
| 3 | 5.658 | 471 | 480 | 495 | rBV | 304979 | 580041 | 45.31% | 6.446% |
| 4 | 7.268 | 747 | 754 | 774 | rBV | 324069 | 642506 | 50.19% | 7.140% |
| 5 | 7.638 | 809 | 817 | 829 | rBV | 351238 | 665848 | 52.02% | 7.399% |
| 6 | 8.108 | 889 | 897 | 908 | rBV | 81195 | 157381 | 12.29% | 1.749% |
| 7 | 8.431 | 944 | 952 | 964 | rBV | 245444 | 482486 | 37.69% | 5.362% |
| 8 | 9.277 | 1088 | 1096 | 1113 | rBV | 174694 | 367317 | 28.69% | 4.082% |
| 9 | 10.928 | 1369 | 1377 | 1388 | rBV | 114460 | 236118 | 18.45% | 2.624% |
| 10 | 13.361 | 1784 | 1791 | 1803 | rBV | 535975 | 892578 | 69.73% | 9.919% |
| 11 | 14.178 | 1924 | 1930 | 1940 | rBV | 200437 | 317747 | 24.82% | 3.531% |
| 12 | 14.742 | 2018 | 2026 | 2037 | rBV2 | 197990 | 357901 | 27.96% | 3.977% |
| 13 | 16.187 | 2267 | 2272 | 2273 | rBV2 | 14389 | 17301 | 1.35% | 0.192% |
| 14 | 16.228 | 2273 | 2279 | 2292 | rVB | 361764 | 633247 | 49.47% | 7.037% |
| 15 | 16.410 | 2306 | 2310 | 2320 | rVB2 | 6977 | 14363 | 1.12% | 0.160% |
| 16 | 17.203 | 2438 | 2445 | 2450 | rBV4 | 9859 | 15684 | 1.23% | 0.174% |
| 17 | 17.486 | 2486 | 2493 | 2505 | rBV | 243176 | 422091 | 32.97% | 4.690% |
| 18 | 17.944 | 2566 | 2571 | 2576 | rBV2 | 13145 | 18296 | 1.43% | 0.203% |
| 19 | 19.753 | 2874 | 2879 | 2885 | rBV | 36505 | 49163 | 3.84% | 0.546% |
| 20 | 20.077 | 2928 | 2934 | 2948 | rBV | 906203 | 1280100 | 100.00% | 14.225% |
| 21 | 20.788 | 3051 | 3055 | 3059 | rVB3 | 28269 | 34965 | 2.73% | 0.389% |
| 22 | 21.363 | 3148 | 3153 | 3162 | rBV4 | 26373 | 59362 | 4.64% | 0.660% |
| 23 | 21.757 | 3213 | 3220 | 3230 | rBV | 253995 | 466112 | 36.41% | 5.180% |
| 24 | 23.220 | 3465 | 3469 | 3479 | rVB10 | 9373 | 21513 | 1.68% | 0.239% |
| 25 | 25.053 | 3767 | 3781 | 3797 | rBV3 | 140853 | 447849 | 34.99% | 4.977% |

Sum of corrected areas: 8999039

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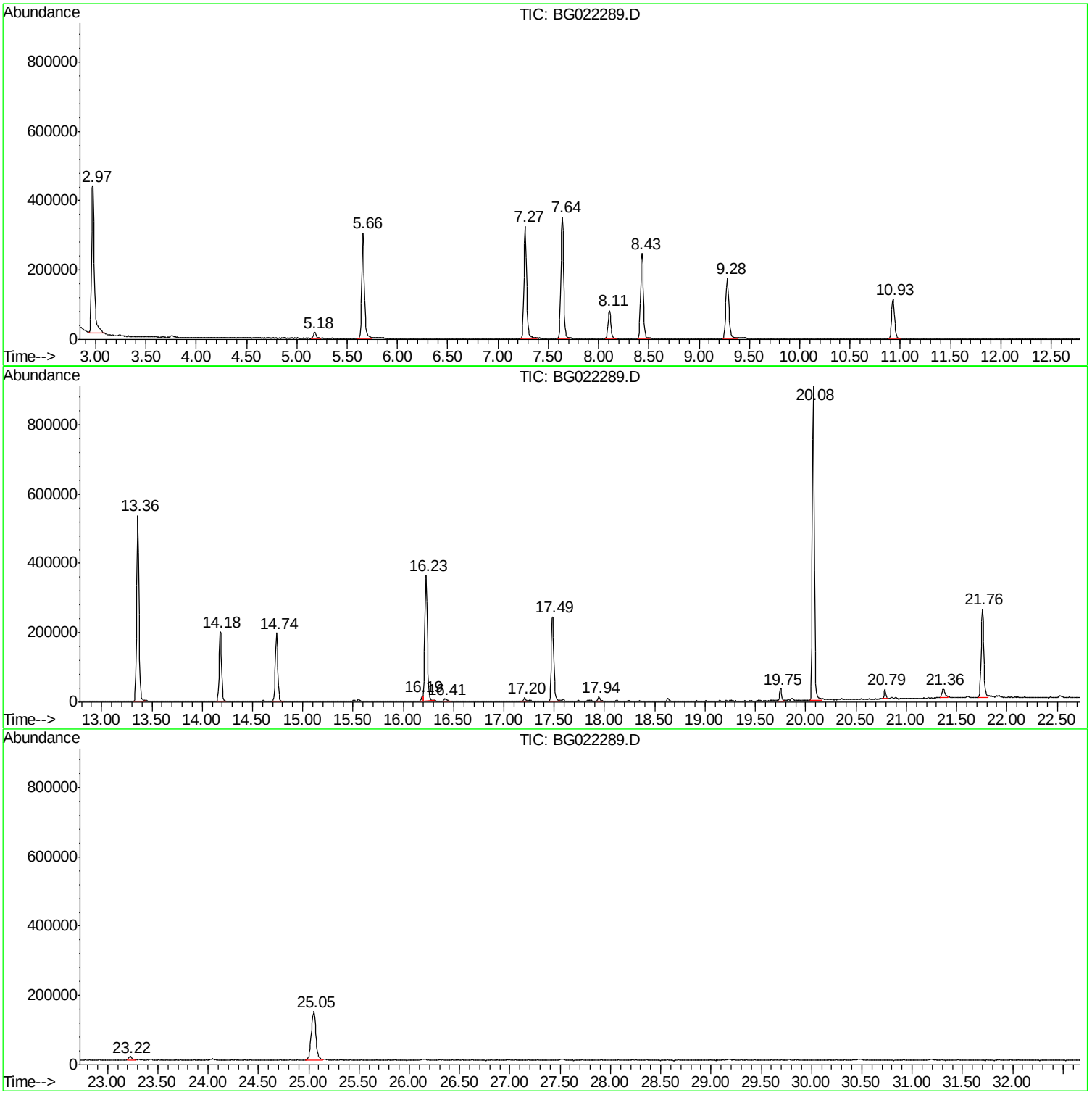
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Acq On : 10 Jun 2016 15:43
Operator : UM/SJ
Sample : H3438-14
Misc :
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**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

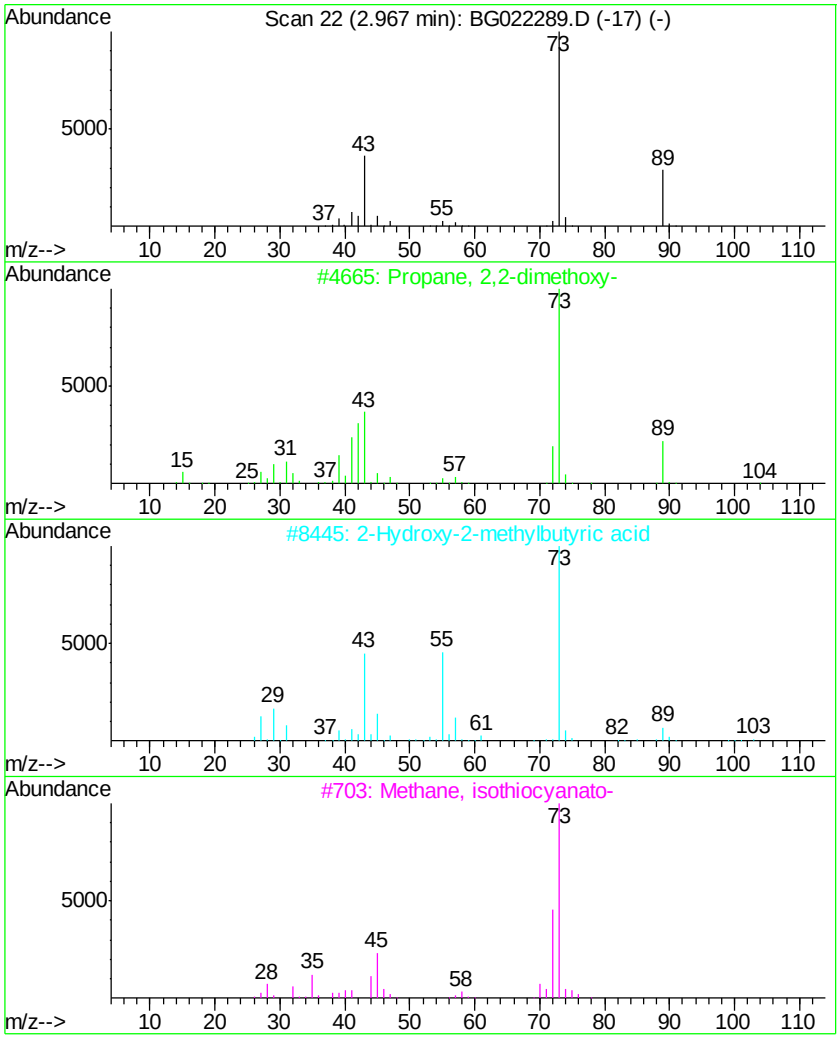
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

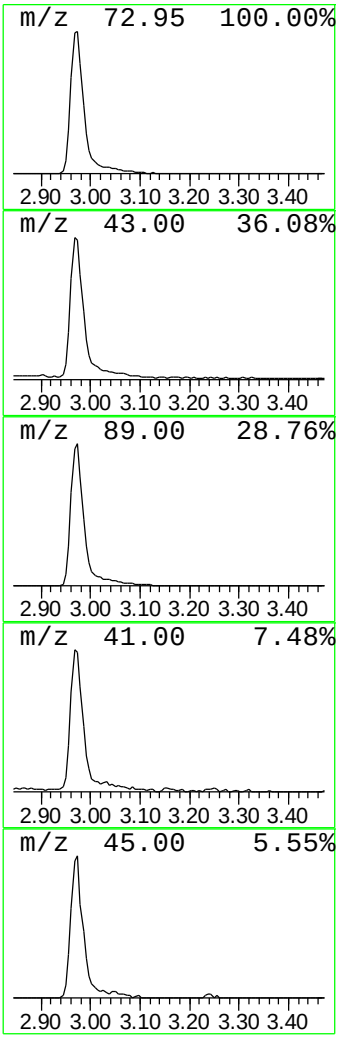
**********

Peak Number 1 unknown2.97 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 2.97 | 99.94 ng | 786455 | 1,4-Dichlorobenzene-d4 | 8.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Propane, 2,2-dimethoxy- | 104 | C5H12O2 | 000077-76-9 | 45 |
| 2 | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 28 |
| 3 | Methane, isothiocyanato- | 73 | C2H3NS | 000556-61-6 | 7 |
| 4 | N-Ethylformamide | 73 | C3H7NO | 000627-45-2 | 7 |
| 5 | 1,3,5-Trioxane | 90 | C3H6O3 | 000110-88-3 | 4 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061016\
Data File : BG022289.D
Acq On : 10 Jun 2016 15:43
Operator : UM/SJ
Sample : H3438-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

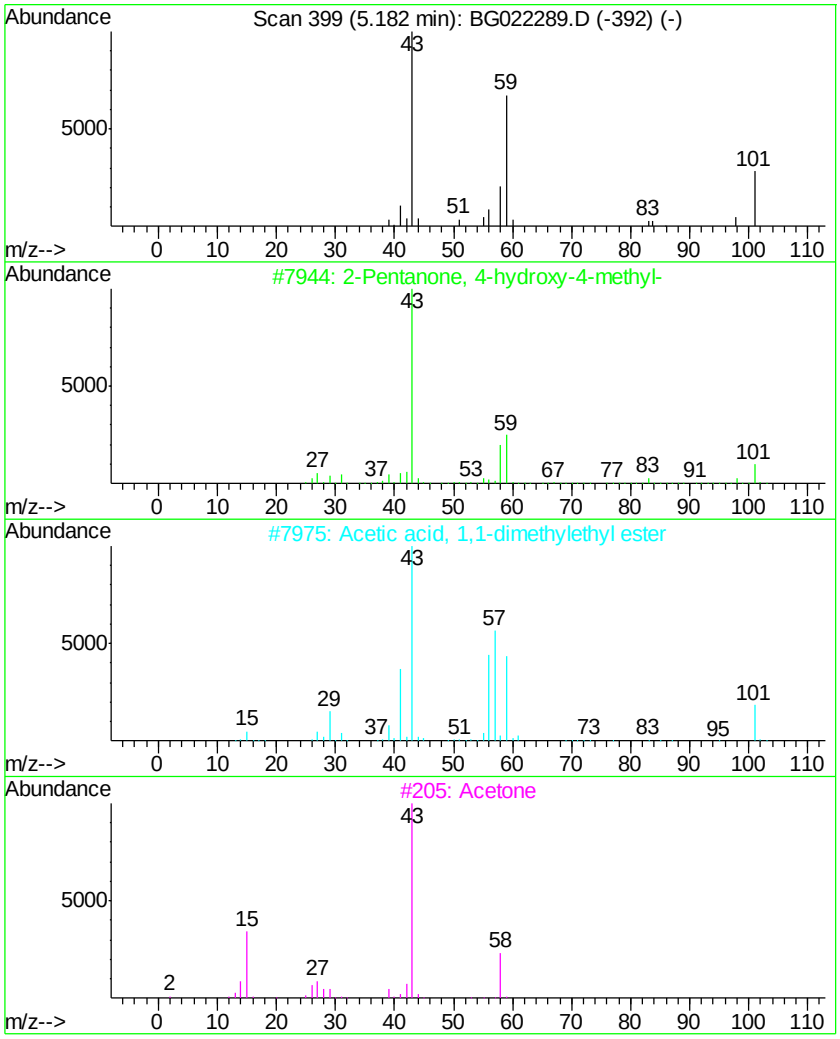
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

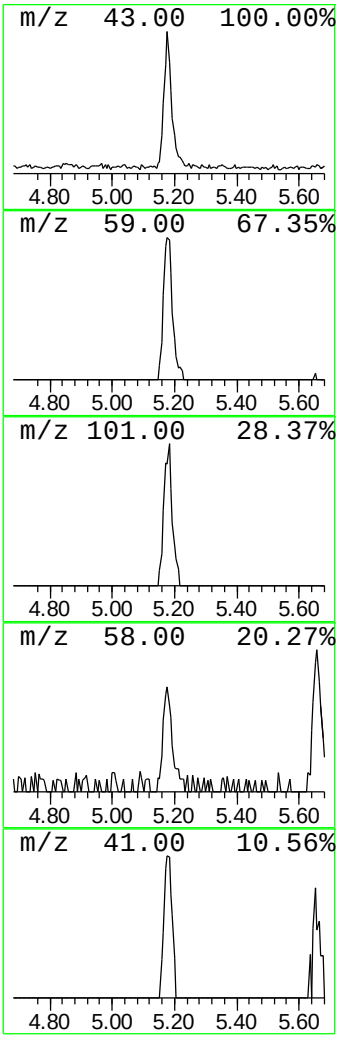
**********

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.18 | 4.14 ng | 32615 | 1,4-Dichlorobenzene-d4 | 8.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53 |
| 2 | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 36 |
| 3 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 4 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 5 | 2-Pentanol, 2,4-dimethyl- | 116 | C7H16O | 000625-06-9 | 9 |



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061016\
Data File : BG022289.D
Acq On : 10 Jun 2016 15:43
Operator : UM/SJ
Sample : H3438-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

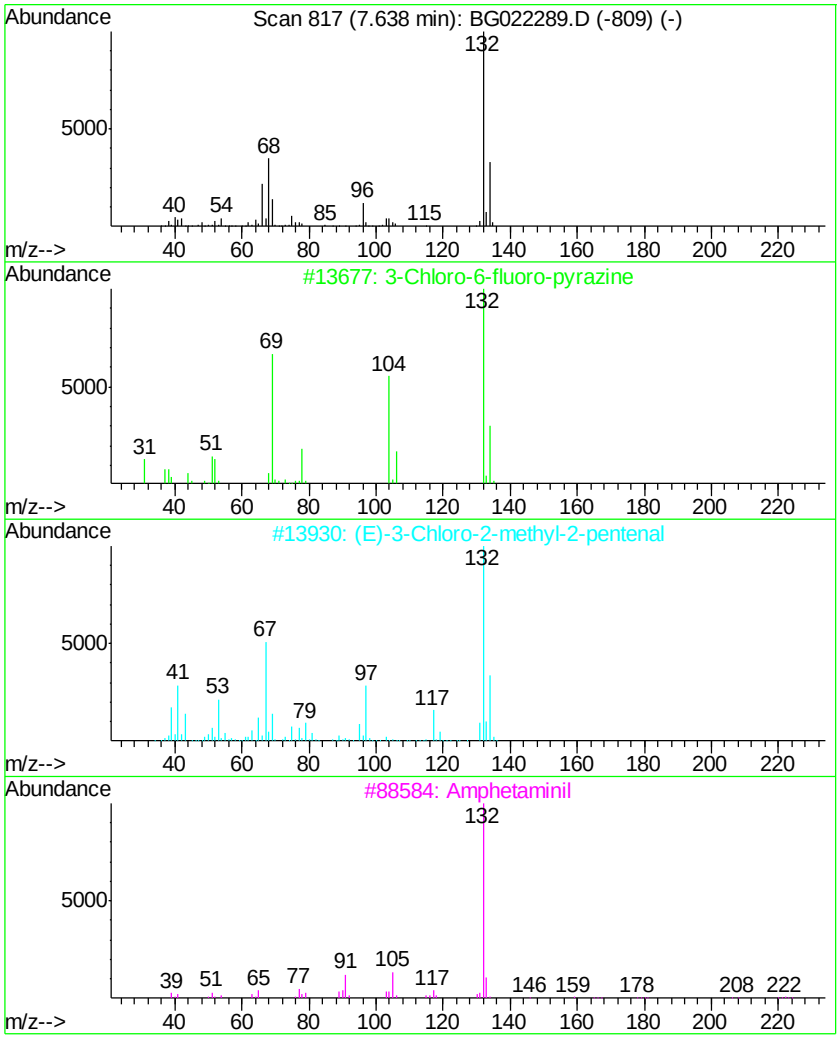
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

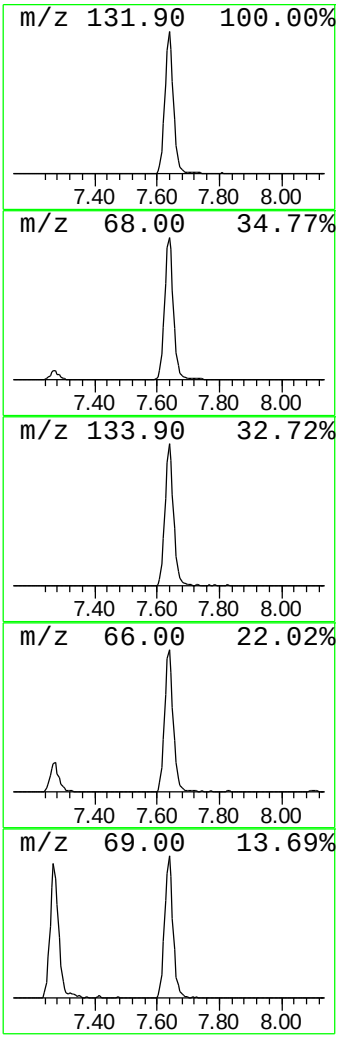
**********

Peak Number 3 unknown7.64 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.64 | 84.62 ng | 665848 | 1,4-Dichlorobenzene-d4 | 8.11 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 38 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 17 |
| 3 | Amphetaminil | 250 | C17H18N2 | 017590-01-1 | 12 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |



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Data File : BG022289.D
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Operator : UM/SJ
Sample : H3438-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

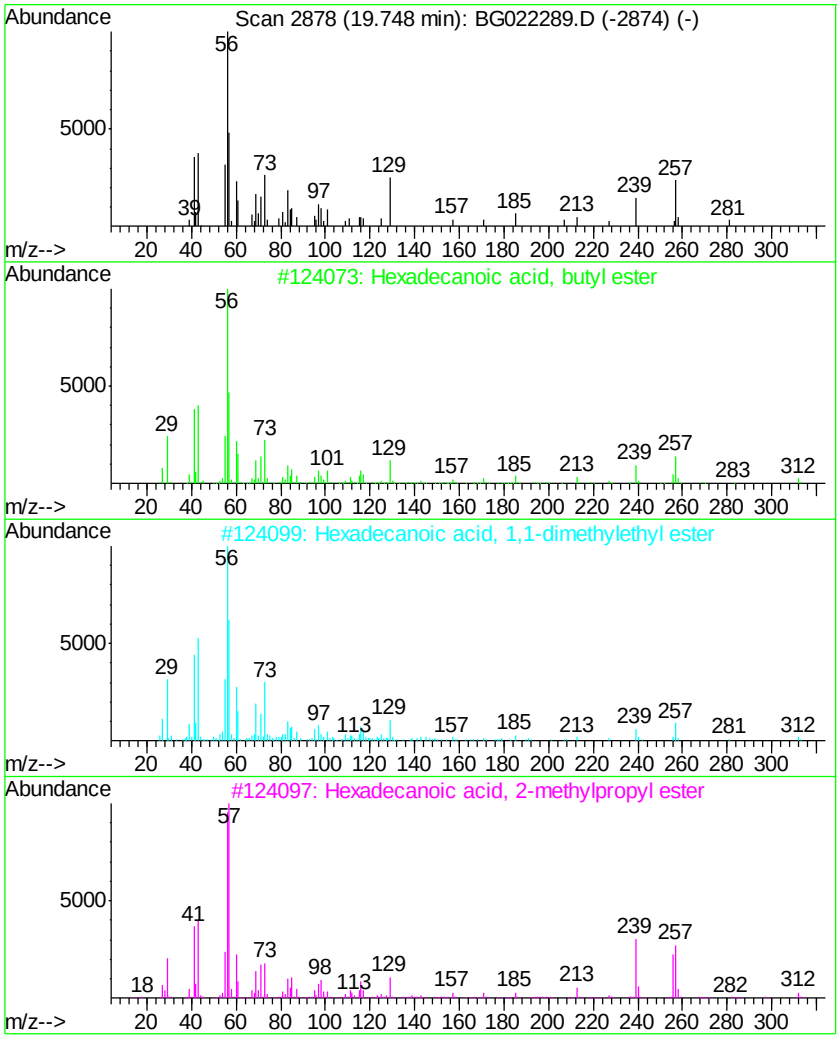
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

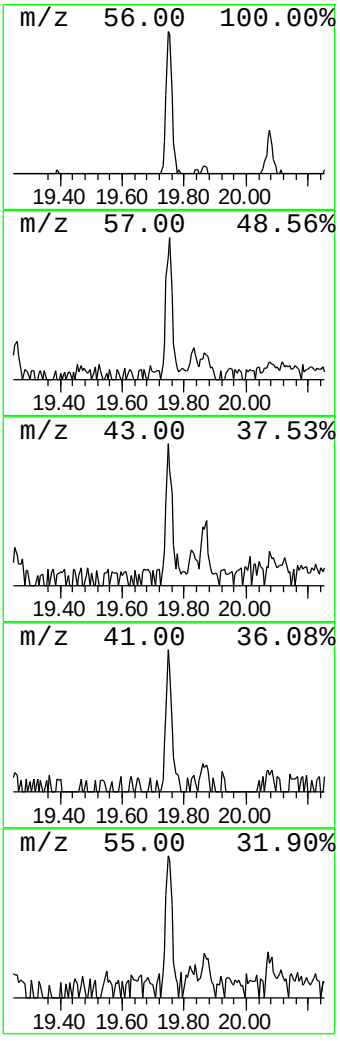
**********

Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.75 | 2.11 ng | 49163 | Chrysene-d12 | 21.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 83 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 74 |
| 3 | Hexadecanoic acid, 2-methylpropy... | 312 | C20H40O2 | 000110-34-9 | 50 |
| 4 | 1-Undecene, 5-methyl- | 168 | C12H24 | 074630-38-9 | 27 |
| 5 | 2-Methyl-1-tetradecene | 210 | C15H30 | 052254-38-3 | 25 |



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Sample : H3438-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

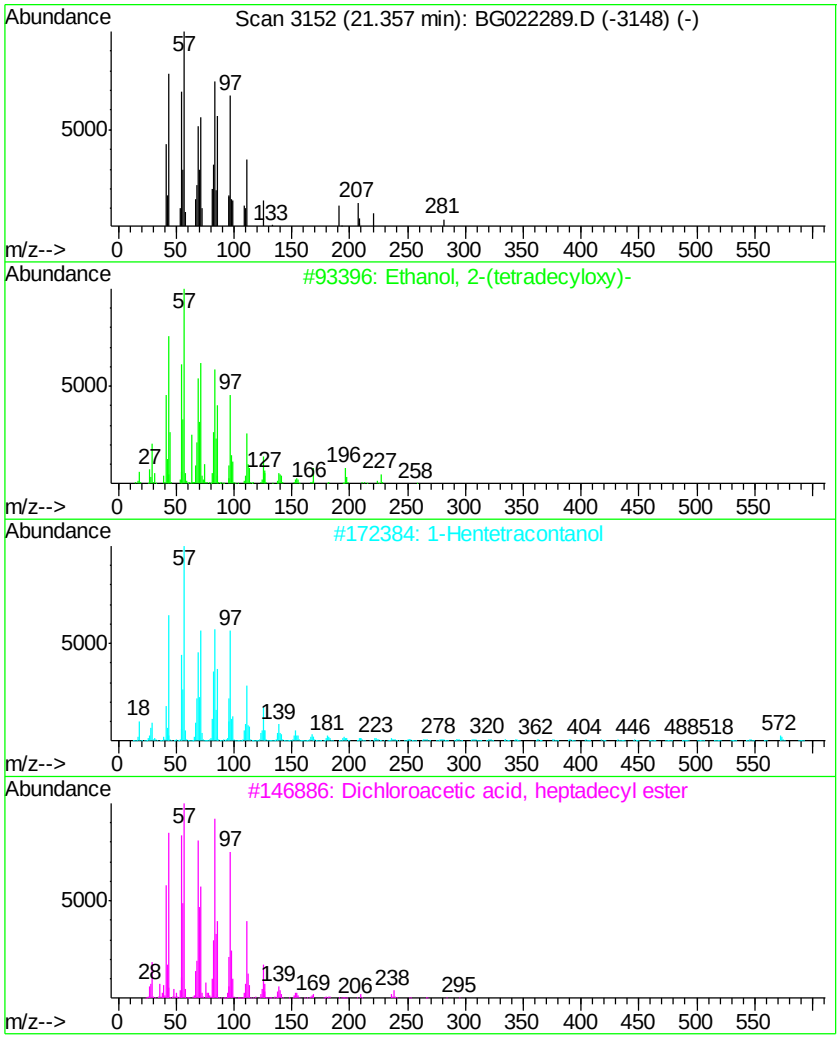
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

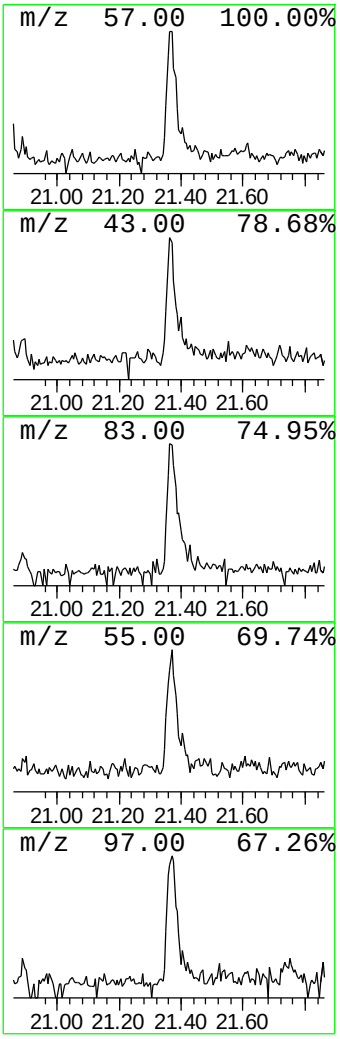
**********

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.36 | 2.55 ng | 59362 | Chrysene-d12 | 21.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanol, 2-(tetradecyloxy)- | 258 | C16H34O2 | 002136-70-1 | 90 |
| 2 | 1-Hentetracontanol | 593 | C41H84O | 040710-42-7 | 87 |
| 3 | Dichloroacetic acid, heptadecyl ... | 366 | C19H36Cl2O2 | 1000282-98-2 | 87 |
| 4 | Octadecane, 1-(ethenyloxy)- | 296 | C20H40O | 000930-02-9 | 86 |
| 5 | 2- Chloropropionic acid, octadec... | 360 | C21H41ClO2 | 088104-31-8 | 83 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061016\
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Misc :
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**Instrument :** BNA_G
**ClientSampleId :** SB-08-COMP

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown2.97 | 2.97 | 99.9 | ng | 786455 | 1 | 8.11 | 157381 | 20.0 |
| 2-Pentanone, 4-hy... | 5.18 | 4.1 | ng | 32615 | 1 | 8.11 | 157381 | 20.0 |
| unknown7.64 | 7.64 | 84.6 | ng | 665848 | 1 | 8.11 | 157381 | 20.0 |
| Hexadecanoic acid... | 19.75 | 2.1 | ng | 49163 | 5 | 21.76 | 466112 | 20.0 |
| Ethanol, 2-(tetra... | 21.36 | 2.5 | ng | 59362 | 5 | 21.76 | 466112 | 20.0 |